

# Rarefied flow modeling in heat battery applications

**Background:** Thermochemical materials (TCMs) have emerged as promising candidates for high-density energy storage, particularly in applications requiring long-term storage with little thermal loss. Vacuum-based reactors are an application of this under development. In this context, the efficient transfer of heat and mass to and from TCMs becomes a critical aspect for the practical deployment of such systems. However, the combination of low pressures and small length scales leads to a collapse of the continuum approximation (Knudsen diffusion), and thus renders traditional continuum based modeling methods invalid, such as the finite volume method (FVM) or the finite element method (FEM).

## Scope:

- **Modeling:** Investigate modeling methods for the transition regime ( $0.1 < Kn < 10$ ), such as the Lattice Boltzmann Method and Direct Simulation Monte Carlo. A method should be chosen and applied to the heat battery case based on considerations such as accuracy, computational cost, and suitability to the case.
- **Micro-CT:** By utilizing micro-CT images it is possible to do direct simulation on the granular morphology at micrometer length scales.
- **Validation:** Compare the results with analytical, empirical and/or other numerical data to validate the results.
- **Optimize:** Investigate how the rarefied flow conditions influence the performance of the heat battery, and test altered morphologies to improve key performance metrics of the heat battery.

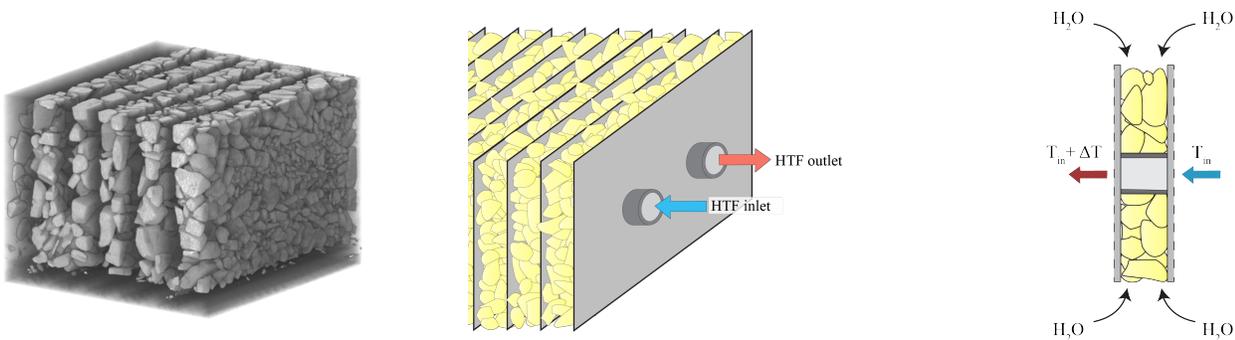


Figure 1: Granular morphology of the TCM in a reactor (left), schematic of the reactor (middle), and working principle of the heat battery (right)

**Candidate profile:** We are in search of a master's student from Mechanical Engineering, Chemical Engineering, or a related field. The ideal candidate has experience with numerical simulations and is proficient in coding. More importantly however, we value curiosity, adaptability, and an interest for leveraging computational methods to advance renewable energy solutions.

## Contact

For more details or to express interest, please contact:

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